

Oxazole
288-42-6 | DTXSID70182983

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 14.3 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.94e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

Image not found

dl-Diepoxybutane

Measured: 11.6

Predicted: 9.80

Image not found

2,2'-Bioxirane

Measured: 11.6

Predicted: 9.80

Image not found

1,3-Dioxolane

Measured: 13.5

Predicted: 11.9

Image not found

1,4-Dioxane

Measured: 11.4

Predicted: 11.2

Image not found

Ethylene oxide

Measured: 22.7

Predicted: 18.1

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1,3-Propylene oxide

Measured: 17.2

Predicted: 11.1